

FAA CENTER OF EXCELLENCE FOR ALTERNATIVE JET FUELS & ENVIRONMENT

# Alternative Jet Fuel Test Database Library

## Project 33

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April 18 & 19, 2019

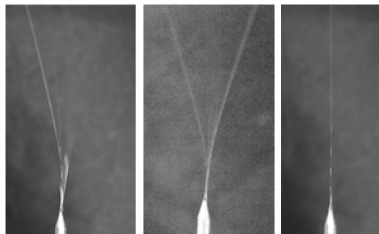
Atlanta, GA

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# My path to alternative jet fuels

- University of Illinois Urbana-Champaign
  - **2012:** *BS ABE* - Hoeft Technology & Management Minor
  - **2014:** *MS MechSE* - Surrogate modeling of alternative jet fuels for study of autoignition characteristics
  - **Current:** *PhD MechSE* – Physicochemical and performance study of next generation alternative jet fuels



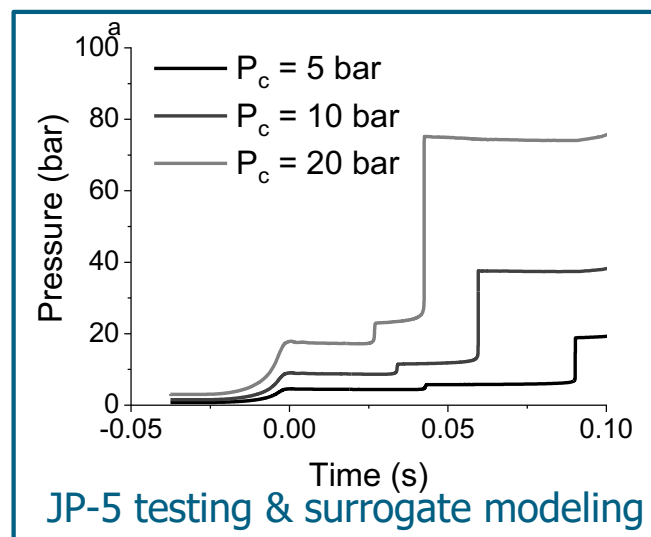
Butanol electrospays



Ionic liquid dissolution of  
lignocellulosic biomass



Algae biofuel & carbon  
sequestration



# Global needs necessitate fuel diversification



Airline travel & commerce doubling over next 20 years<sup>1</sup>



CORSIA CO<sub>2</sub> mandate 2019  
2050 target  
-50% CO<sub>2</sub>



Fuel sourcing instability & market volatility  
3000+ fuel convoy deaths 2003-2007<sup>2</sup>

<sup>1</sup>International Air Transport Association (IATA) Press Release No. 62, 2018

<sup>2</sup>Army Environmental Policy Institute, Sustain the Mission Project: Casualty Factors for Fuel and Water Supply Convoys 2009

# Address three critical facets for AJF expansion & integration



***Alternative Jet  
Fuel Development  
& Deployment***

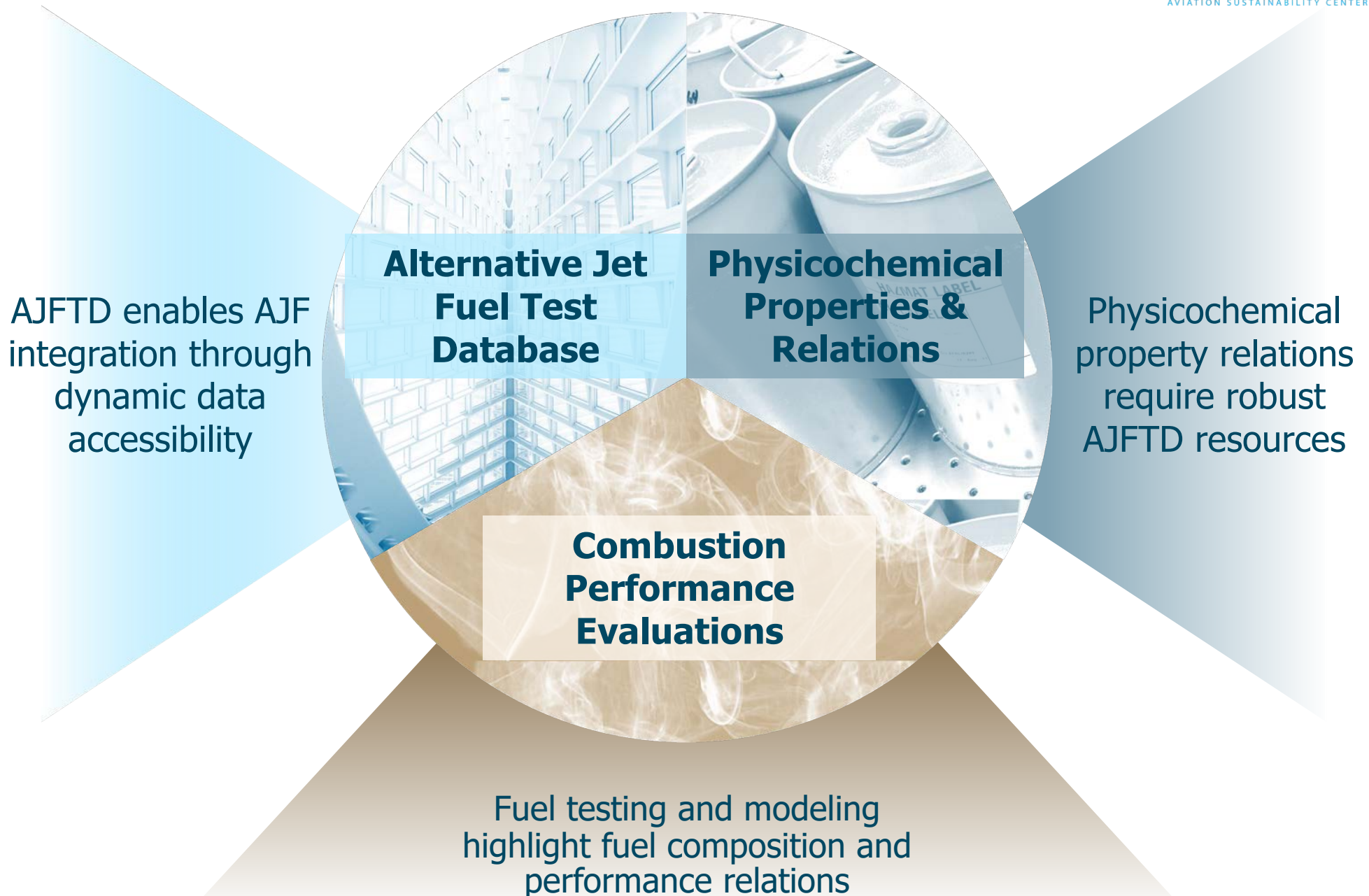
**Alternative Jet  
Fuel Test  
Database**

**Physicochemical  
Properties &  
Relations**

**Combustion  
Performance  
Evaluations**



# Support continued AJF development & deployment



# Alternative Jet Fuels Test Database



***Foundational database of current  
& emerging alternative jet fuels***

## Goals:

- **Compile jet fuel data** into comprehensive, centralized knowledgebase
- **Integrate knowledge on AJF development** path to aid in design and certification of new jet fuels
- **Support alternative fuels research** and certification for national and international multi-stakeholder initiatives
- **Increase accessibility** to fuel testing data and approval reporting

# Focus on critical fuel property & test data



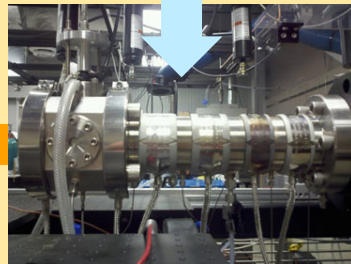
Feedstock  
production &  
logistics



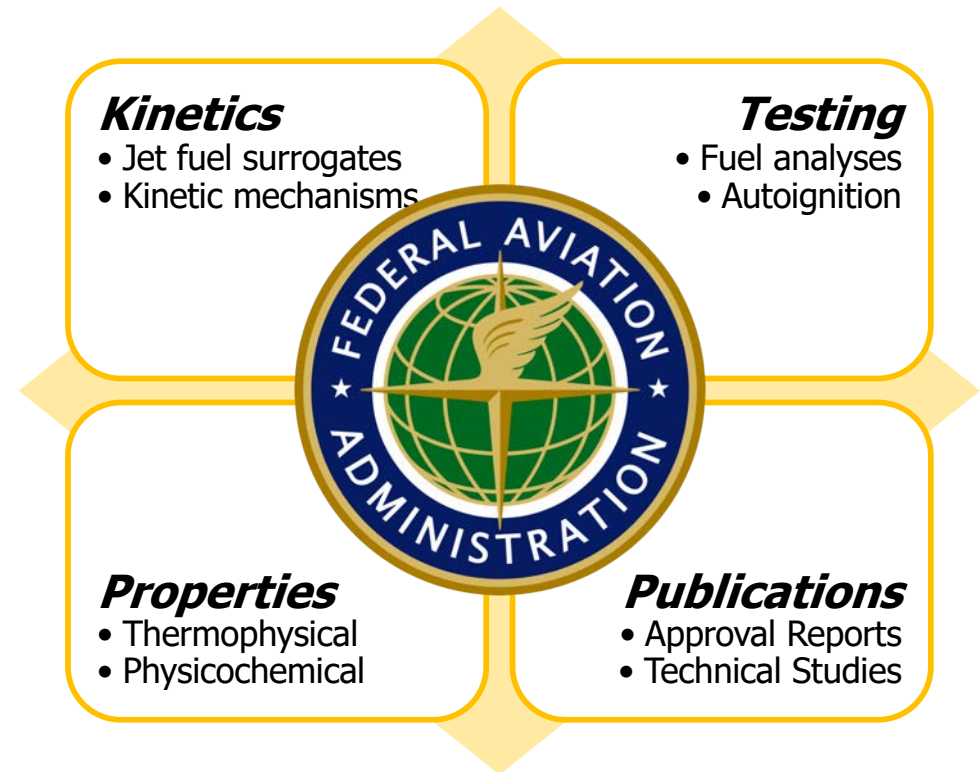
Conversion,  
scale-up &  
processing



End use production  
& emission testing



Fuel property  
testing &  
approval



# AJFTD annual targets & tasks



*Year 1*

- Identify available ***data resources*** - collect fuel test data

*Year 2*

- Develop ***web interface*** - optimize data schema and populate database

*Year 3*

- Understand ***AJF variability*** - evaluate tools for fuel blend property predictions

*Year 4*

- Expand ***analysis capabilities*** and ***data storage*** - convert fuel data for enhanced integration

*Year 5*

- Upgrade site to directly and ***dynamically interface*** with database  
- extract useful fuel statistics (e.g. category distributions)



# Fuel property & test data sources



## Air Force Research Lab (AFRL)

- 400+ POSF numbers
- GCxGC data for 87 fuels

## Petroleum Quality Information Systems (PQIS)

- 9,201 fuel records

## Metron Aviation

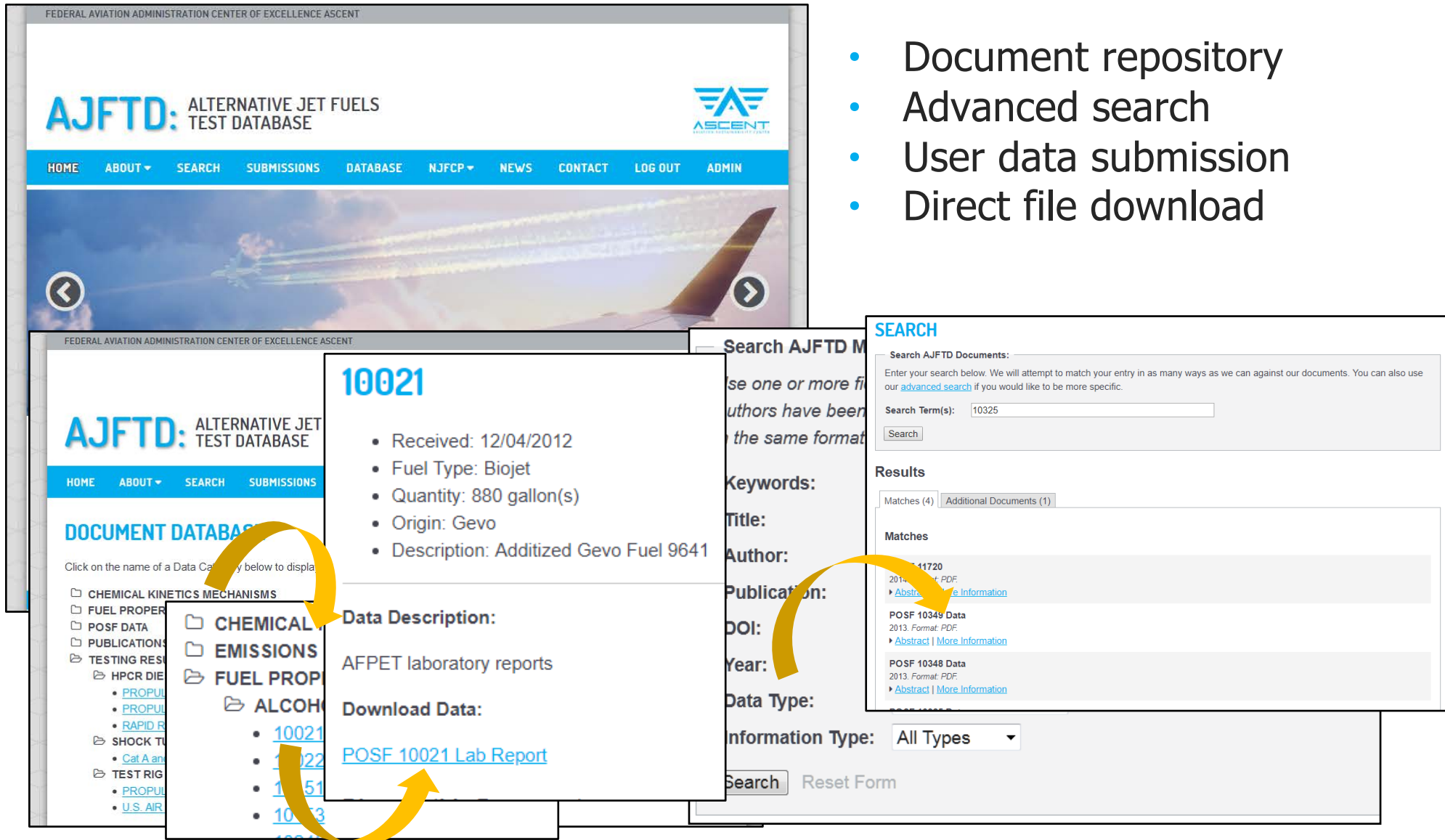
- 14,823 fuel records across 13 domestic airports

## NJFCP

- Fuel property and test data for Category A and C fuels

# Gen I: user specified queries & file download

- Document repository
- Advanced search
- User data submission
- Direct file download



The screenshot displays the AJFTD (Alternative Jet Fuels Test Database) website interface. The main header includes the AJFTD logo and navigation links: HOME, ABOUT, SEARCH, SUBMISSIONS, DATABASE, NJFCP, NEWS, CONTACT, LOG OUT, and ADMIN. The main content area features a large image of a jet engine and a search bar. Below the search bar, there is a section for 'DOCUMENT DATABASE' with a list of categories: CHEMICAL KINETICS MECHANISMS, FUEL PROPERTIES, POSF DATA, PUBLICATIONS, TESTING RESULTS, HPCR DIE, SHOCK TUBE, TEST RIG, and U.S. AIR FORCE. A yellow arrow points from the 'FUEL PROPERTIES' category to a detailed view of document 10021. This view shows the document's metadata: Received: 12/04/2012, Fuel Type: Biojet, Quantity: 880 gallon(s), Origin: Gevo, and Description: Additized Gevo Fuel 9641. A yellow arrow points from the 'Download Data' section to the 'POSF 10021 Lab Report' link. Another yellow arrow points from the 'Search' section to the 'Search AJFTD Documents' form, which includes a search term input field and a search button. The search results show matches for 'POSF 10349 Data' and 'POSF 10348 Data'.

**AJFTD: ALTERNATIVE JET FUELS TEST DATABASE**

HOME ABOUT SEARCH SUBMISSIONS DATABASE NJFCP NEWS CONTACT LOG OUT ADMIN

**DOCUMENT DATABASE**

Click on the name of a Data Category below to display its contents.

- CHEMICAL KINETICS MECHANISMS
- FUEL PROPERTIES
- POSF DATA
- PUBLICATIONS
- TESTING RESULTS
- HPCR DIE
- SHOCK TUBE
- TEST RIG
- U.S. AIR FORCE

**10021**

- Received: 12/04/2012
- Fuel Type: Biojet
- Quantity: 880 gallon(s)
- Origin: Gevo
- Description: Additized Gevo Fuel 9641

**Data Description:**

AFPET laboratory reports

**Download Data:**

[POSF 10021 Lab Report](#)

**Search AJFTD Documents:**

Enter your search below. We will attempt to match your entry in as many ways as we can against our documents. You can also use our [advanced search](#) if you would like to be more specific.

Search Term(s):

**Results**

Matches (4) | Additional Documents (1)

**Matches**

- POSF 11720  
2013. Format: PDF.  
[Abstract](#) | [More Information](#)
- POSF 10349 Data  
2013. Format: PDF.  
[Abstract](#) | [More Information](#)
- POSF 10348 Data  
2013. Format: PDF.  
[Abstract](#) | [More Information](#)

**Keywords:**

**Title:**

**Author:**

**Publication:**

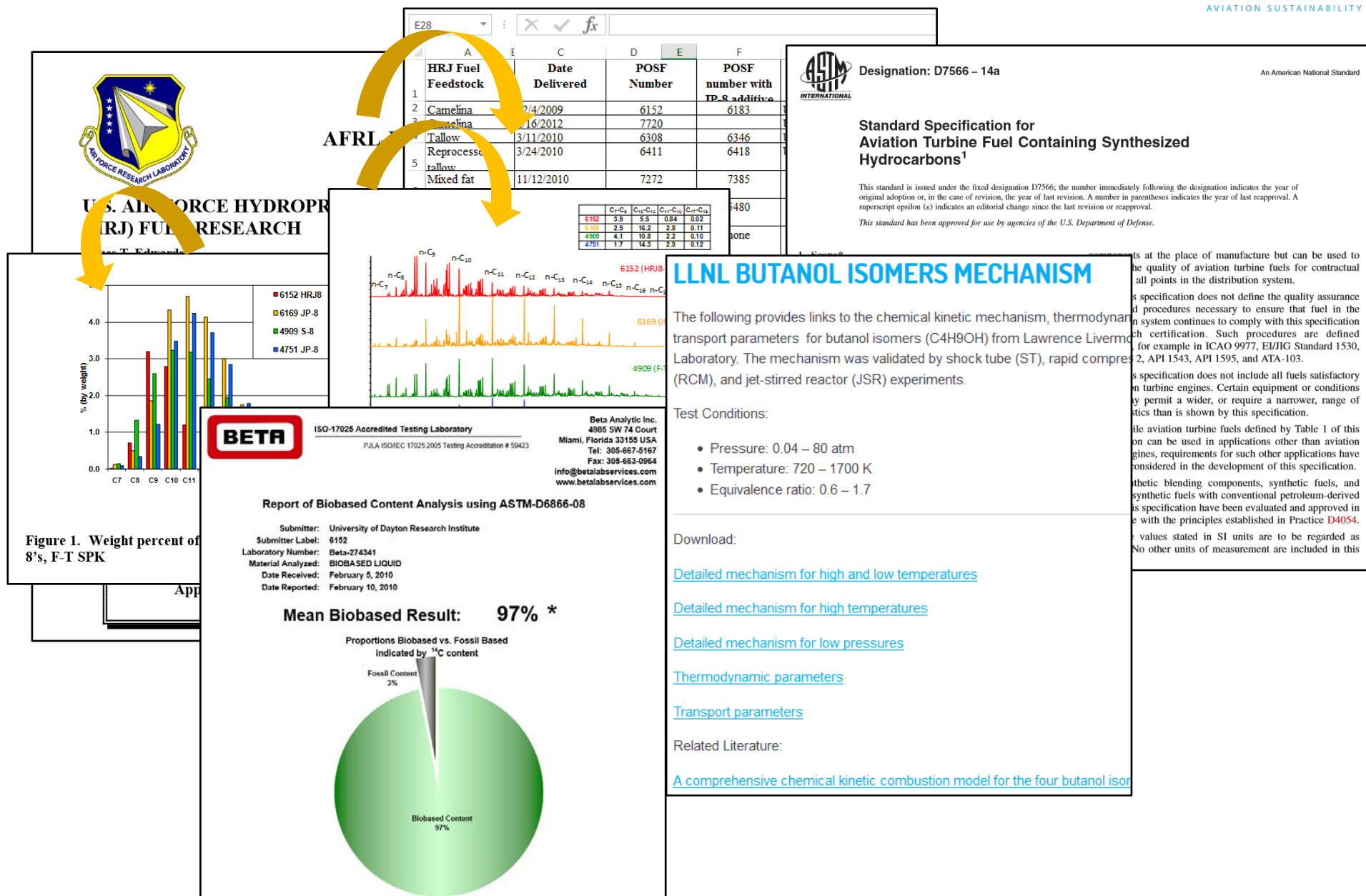
**DOI:**

**Year:**

**Data Type:**

**Information Type:**

# Centralized data resource



# Data conversion incentives



- Accelerate **data retrieval**
  - Easily find fuels without searching hundreds of reports
- Enable **statistical analyses**
  - Develop correlations for global combustion properties
  - Expanded dataset provides more meaningful and robust correlations
- Identify **unusual data** (misreported, outliers, ...)
- **Facilitate collaboration** with related programs and data sharing (JETSCREEN)

# Adaptable NoSQL data structure



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## *Non-Relational (NoSQL)*

### **Flexible schema**

variable data can be easily  
inserted/alterd

---

## *Relational (SQL)*

### **Structured schema**

new data must be consistent with  
predefined structure

---

## ***DynamoDB***

- ✓ AWS @ Illinois partnership
- ✓ University maintained – minimize liability, unintended costs
- ✓ Connect with databases using JSON format documents



# Encapsulate variable information

**Report PDF**

Wright  
01 Date  
Date  
Case Sample No: 12011  
JON: GENERAL FUND

Sample Submitter:  
AFRL/RQTF  
1790 Loop Road N  
Bldg 490  
Wright-Patterson AFB, OH 45433

Reason for Submission: AFRL Research  
Product: Aviation Turbine Fuel, Kerosene  
Specification: MIL-DTL-5624V Grade:JP-5

Qty Submitted: 2 gal

**Excel**

	A	B
1	Method	Test
2	MIL-STD-3004C(1)	Appearance
3	ASTM D 6045 - 12	Color, Saybolt
4	ASTM D 3242 - 11	Total Acid Number (mg KOH/g)
5	ASTM D 1319 - 14	Aromatics (% vol)
6	ASTM D 3227 - 13	Mercaptan Sulfur (% mass)
7	ASTM D 4294 - 10	Total Sulfur (% mass)
8	ASTM D 86 - 12	Distillation
9		Initial Boiling Point (°C)
10		10% Recovered (°C)
11		20% Recovered (°C)
12		50% Recovered (°C)
13		90% Recovered (°C)
14		End Point (°C)

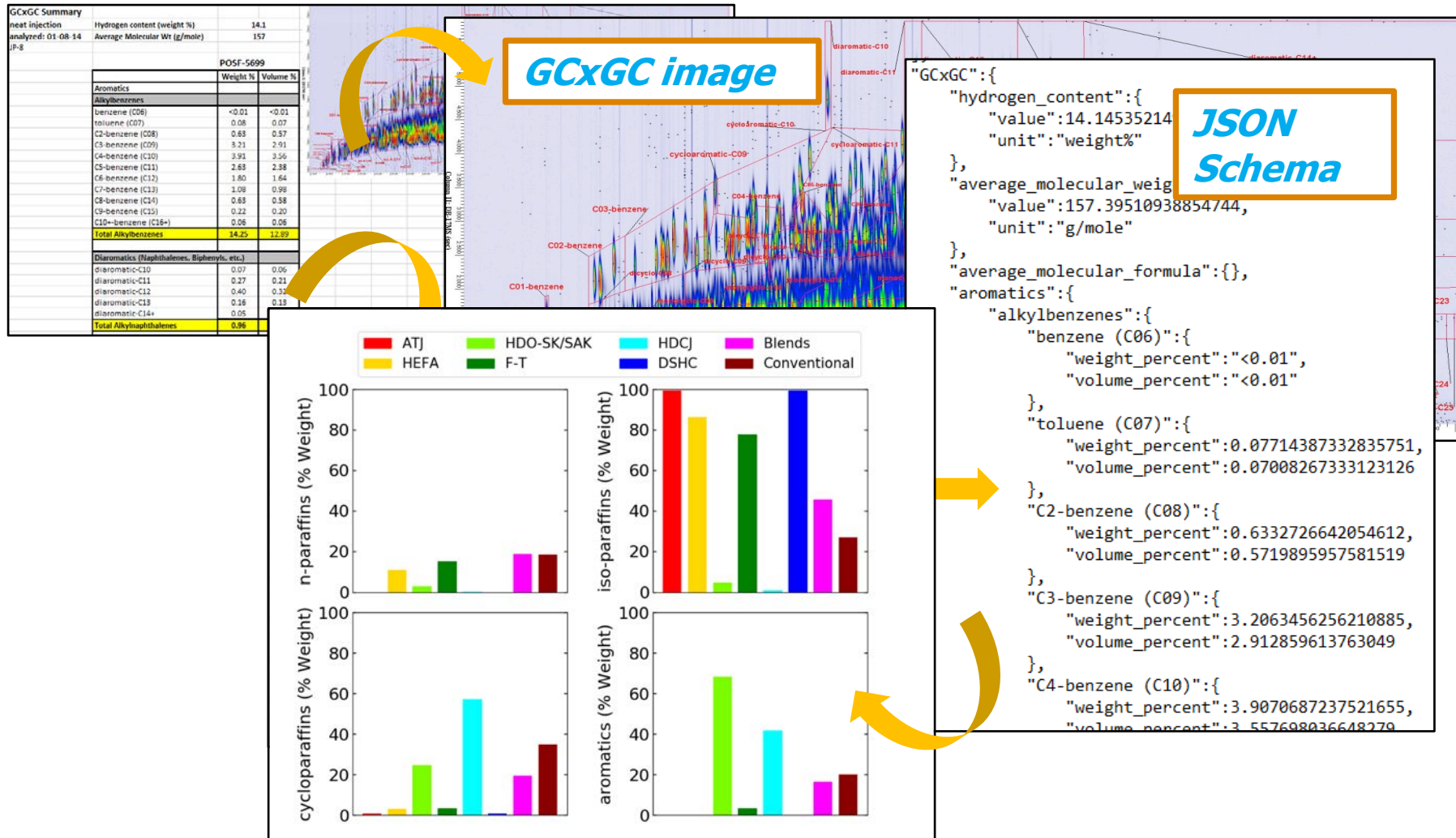
**JSON**

```
"distillation": [
  {
    "volume_evaporated_value": 0,
    "test_method": "D 86",
    "maximum_value": "",
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  },
  {
    "volume_evaporated_value": "10",
    "test_method": "D 86",
    "maximum_value": 205.0,
    "value": 204,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": ""
  },
  {
    "volume_evaporated_value": "20",
    "test_method": "D 86",
    "maximum_value": "",
    "value": 212,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  },
  {
    "volume_evaporated_value": "20",
    "test_method": "D 86",
    "maximum_value": "",
    "value": 212,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  },
  {
    "volume_evaporated_value": "230",
    "test_method": "D 86",
    "maximum_value": "",
    "value": 230,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  },
  {
    "volume_evaporated_value": "245",
    "test_method": "D 86",
    "maximum_value": "",
    "value": 245,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  },
  {
    "volume_evaporated_value": "300",
    "test_method": "D 86",
    "maximum_value": "",
    "value": 300,
    "volume_evaporated_unit": "%",
    "time_stamp": "15/03/13 13:01",
    "unit": "C",
    "minimum_value": "Report Only"
  }
]
```

Method	Test	Min	Max	Result	F
MIL-STD-3004C(1)	Appearance			Pass	
ASTM D 6045 - 12	Color, Saybolt	Report Only		+18	
ASTM D 3242 - 11	Total Acid Number (mg KOH/g)		0.015	0.002	
ASTM D 1319 - 14	Aromatics (% vol)		25.0	11.2	
ASTM D 3227 - 13	Mercaptan Sulfur (% mass)		0.002	0.000	
ASTM D 4294 - 10	Total Sulfur (% mass)		0.30	0.02	
ASTM D 86 - 12	Distillation				
	Initial Boiling Point (°C)	Report Only		183	
	10% Recovered (°C)		205	204	
	20% Recovered (°C)	Report Only		212	
	50% Recovered (°C)	Report Only		230	
	90% Recovered (°C)	Report Only		245	
	End Point (°C)		300	256	

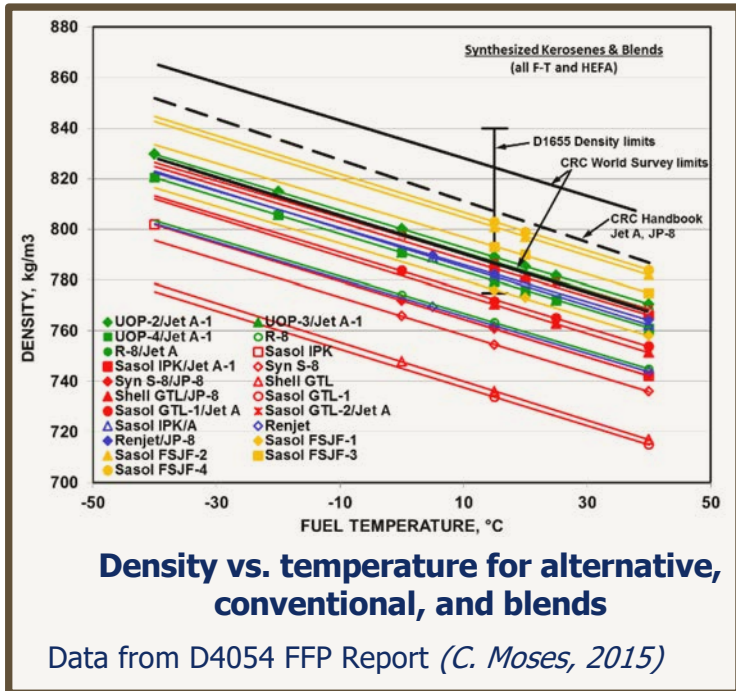
25,000+ fuel records converted to flexible JSON schema

# Unify disparate data formats



Site enables enhanced fuel comparison capabilities

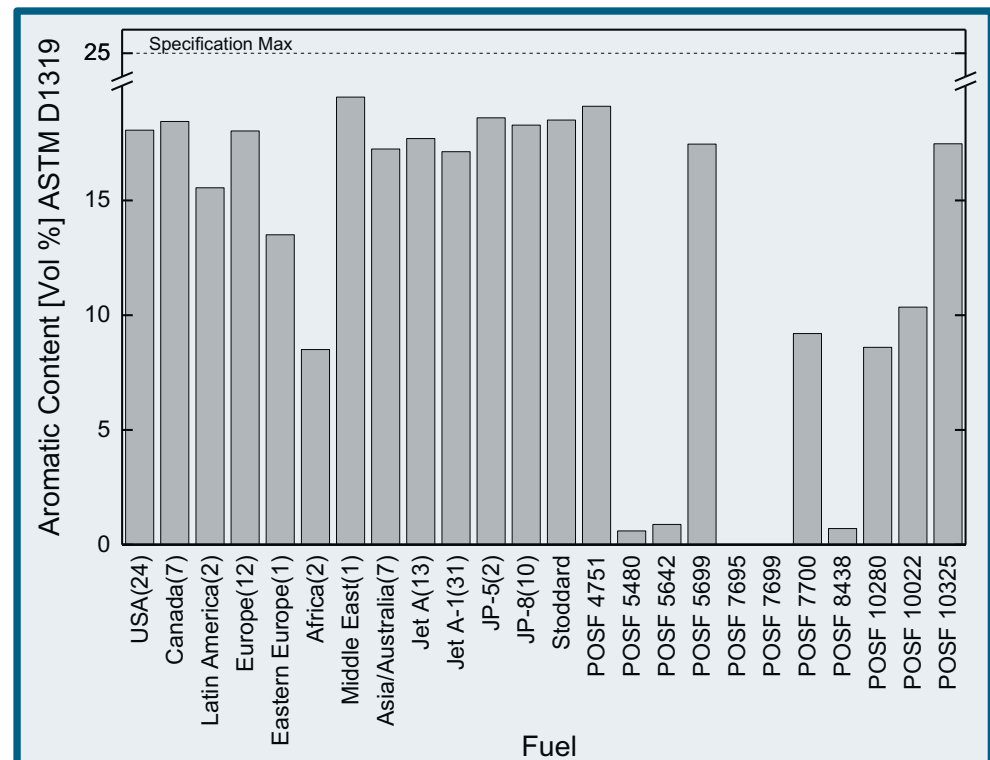
# Enable fuel property evaluations



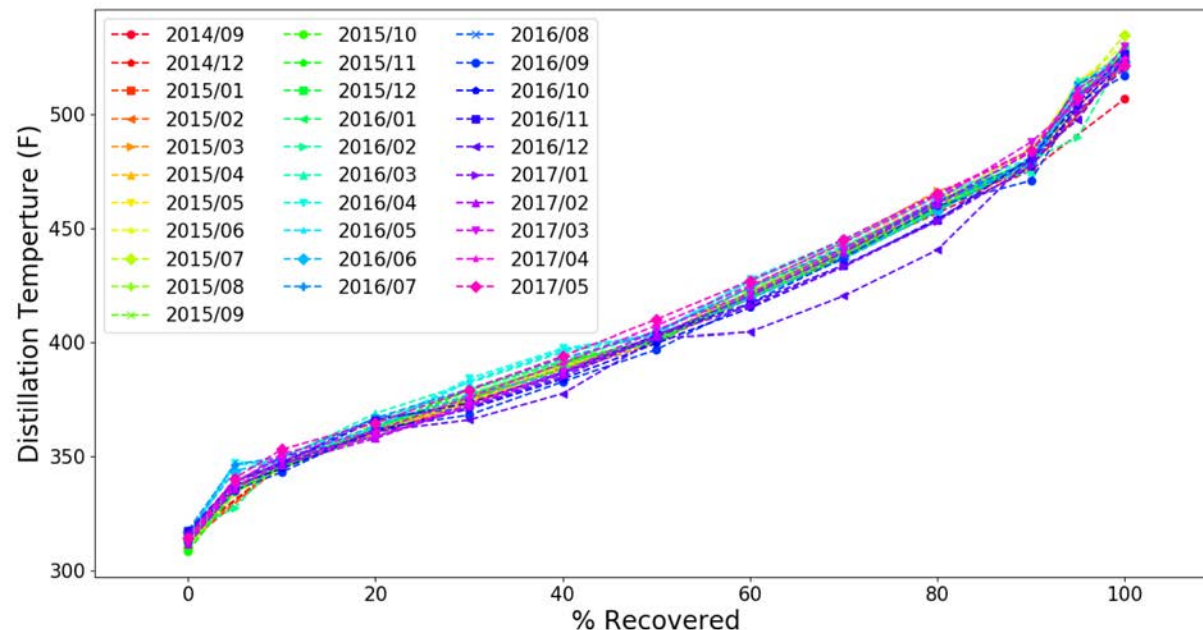
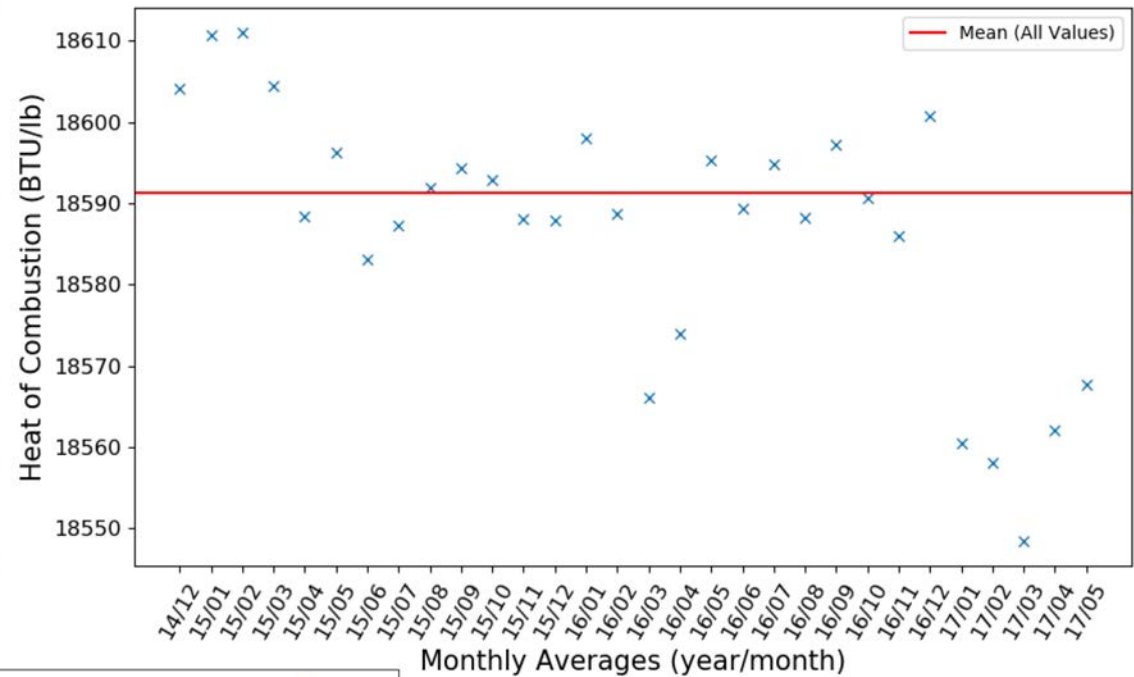
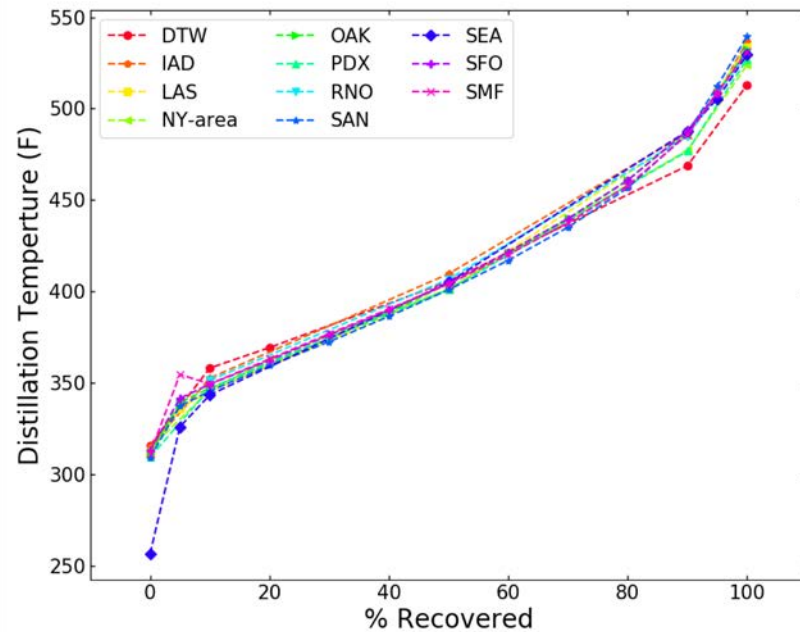
Property	Fuel Type Variance
Density	SKA
Isentropic Bulk Modulus	HEFA, FT
Specific Heat	FT, FSJF
Speed of Sound	HEFA
Viscosity	SKA, HEFA

Surface Tension	Equation
WFS	$y = -0.0751x + 27.4$
FT & HEFA	$y = -0.0741x + 25.9$
SPK	$y = -0.0800x + 25.9$
Renewables	$y = -0.0771x + 26.7$
CRC	$y = -0.0443x + 16.0$

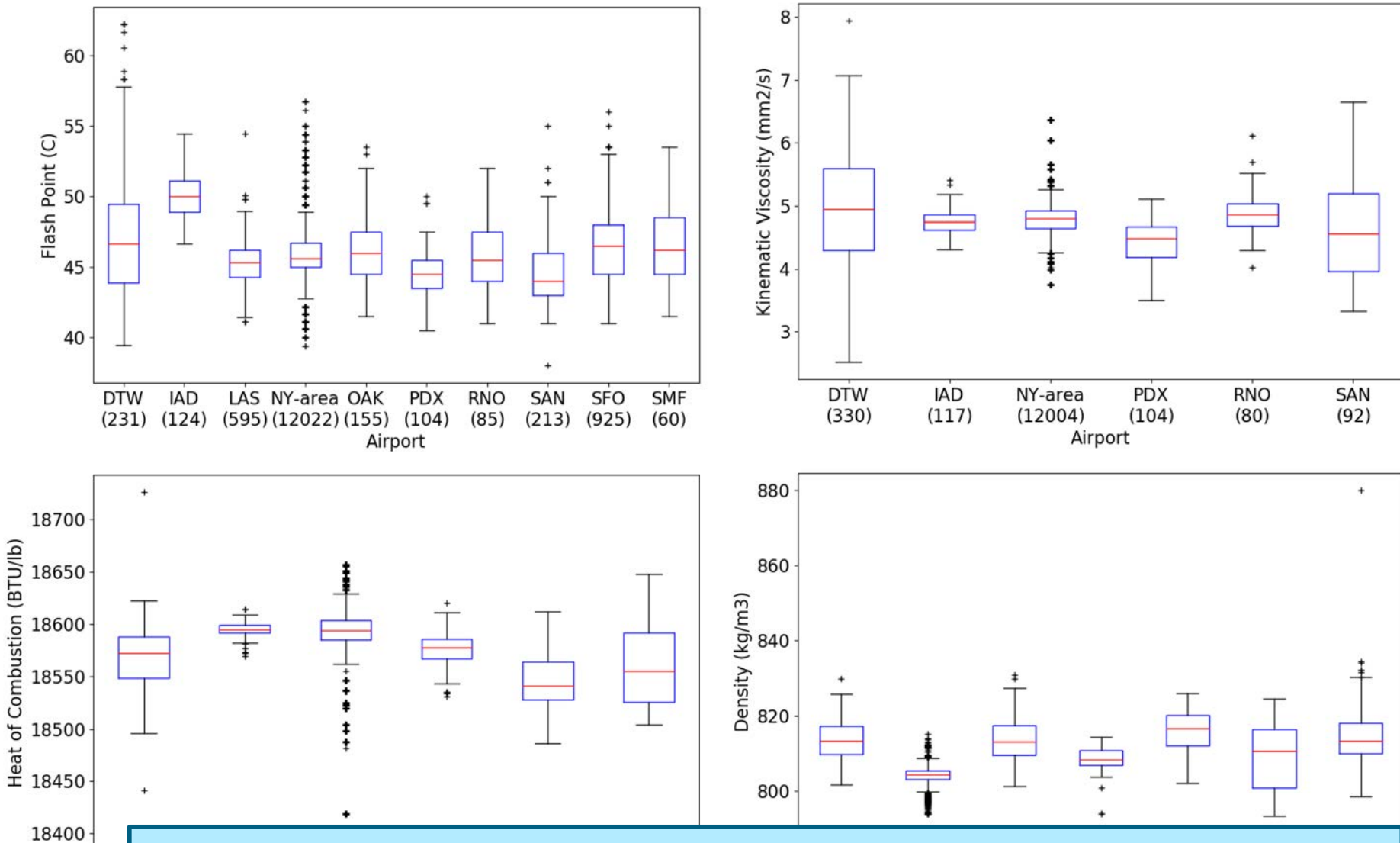
- ❖ Analyzed AJF variance from D4054 FFP report
  - Found significant slope variance in all property categories except surface tension
- ❖ Generated thermophysical relations and specification property value ranges
- ❖ Extended CRC WFS report with AJFTD data
  - Compared conventional fuels against AJFs for various specification requirements



# Domestic airport data highlight reporting inconsistencies



# Airport COA data demonstrate need for testing standardization



Fuel distributions elucidate data recording challenges



# Composition-property evaluations elucidate property dependency

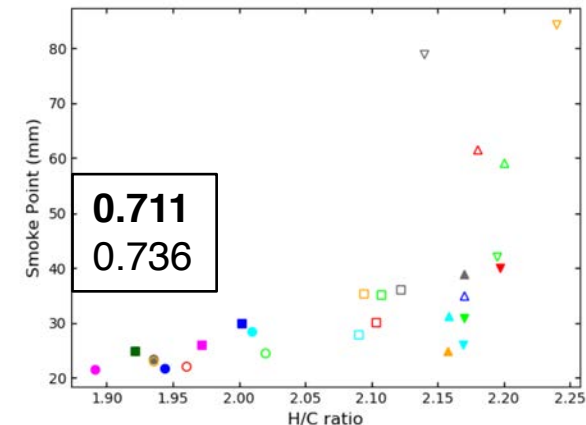
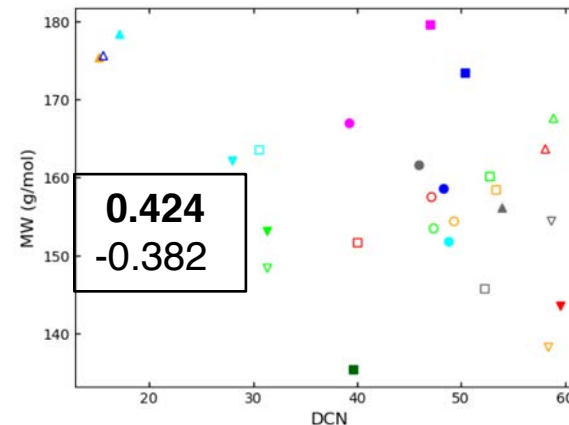
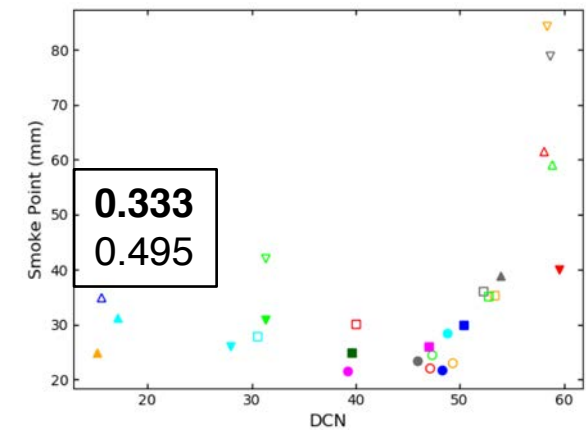
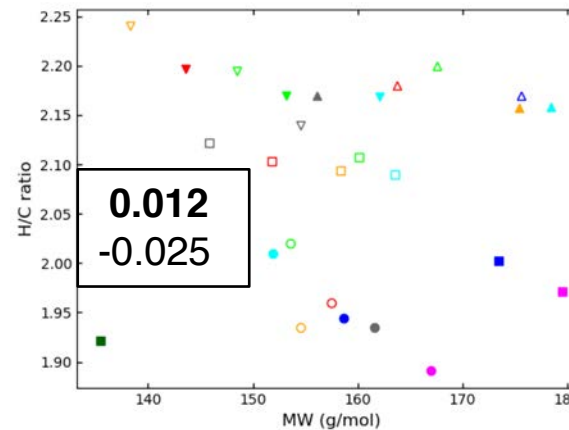
Select fuel properties: DCN, MW, H/C ratio, SP



Evaluate property correlations



Eliminate dependent properties



H/C:SP dependency indicates specification redundancy

# Multiple Linear Regression employs reduced independent property set

$$y_{MLR} = \beta_0 + \beta_1 CP_{DCN} + \beta_2 CP_{H/C} + \beta_3 CP_{MW}$$

Combustion Properties			Selected Fuel Properties		
DCN	H/C Ratio	MW [g/mol]	Flash Point [°C]	Freezing Point [°C]	Net Heat of Combustion [MJ/kg]
Training Set – fuels across conventional, AJF, and blends					

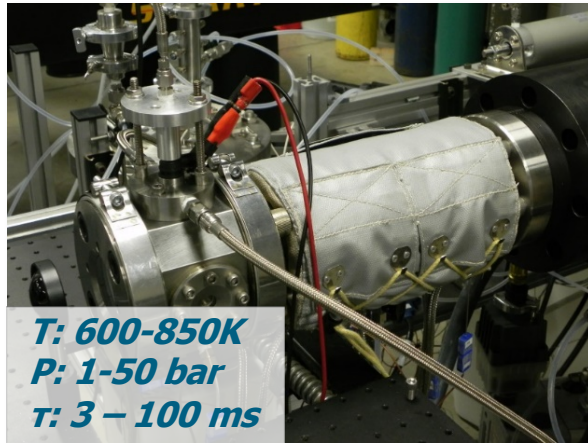
Fuel Property	$\beta_0$	$\beta_1$	$\beta_2$	$\beta_3$
Flash Point	34.12	0.1497	-25.92	0.3902
Freezing Point	16.80	0.4877	-49.17	0.0346
Net Heat of Combustion	35.34	0.003780	3.635	0.003568
Kinematic Viscosity	-10.14	0.004741	-0.5214	0.0942

Testing Set Fuel Type	MLR % Error		
	Flash Point [°C]	Freezing Point [°C]	Net Heat of Combustion [MJ/kg]
Conventional	4.65	8.82	0.00
SPK	2.65	7.73	0.51
Conventional	6.41	3.08	0.79
Conventional	5.99	8.26	0.63
Blend	4.74	5.04	0.07
Renewable	1.84	5.28	0.84

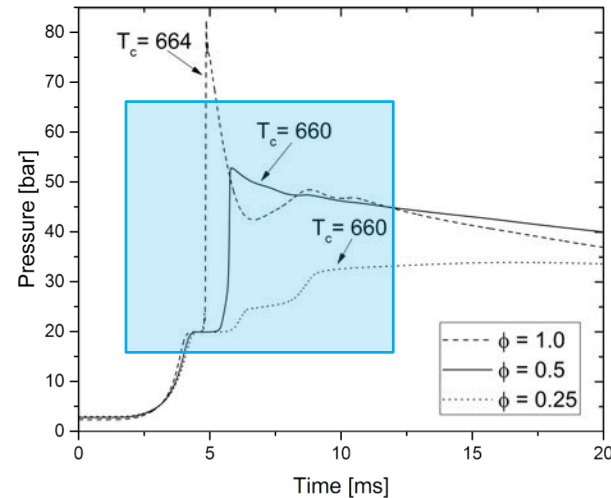
Advances prior studies on limited conventional datasets

# Testing focuses on unique autoignition reactivity

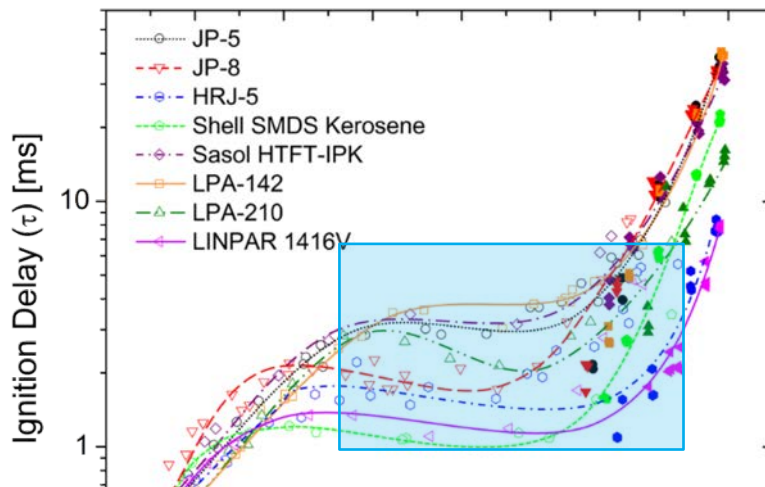
*Rapid Compression Machine (RCM)*



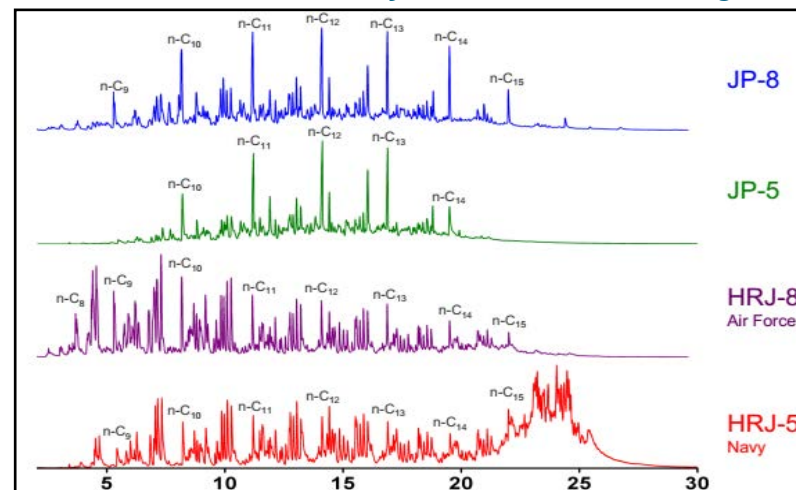
*Equivalence ratio effect on ignition profile*



*Ignition delay trends with NTC region highlighted*



*Conventional and alternative jet fuel total ion chromatograms*



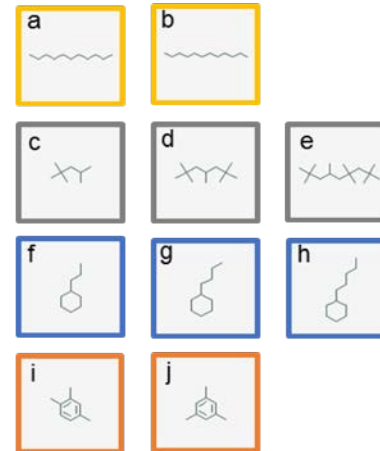
Reaction routes diverge at edges of operational envelope

# F-24 & Gevo testing address fuel blending performance impact

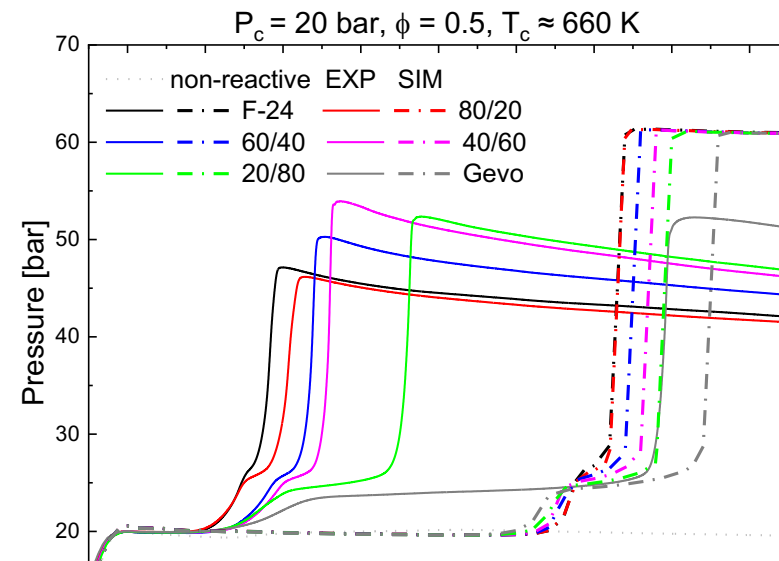
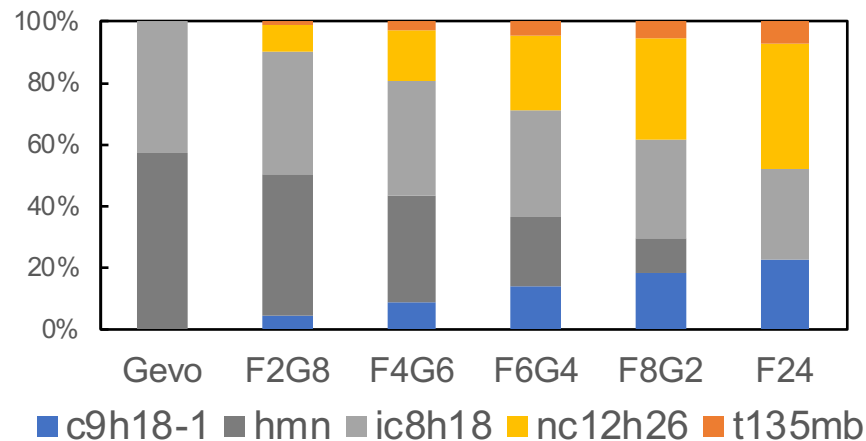
Surrogate species descriptions

Class	Species	Formula	Full name	Figure ID
n-alkane	nC11H24	C11H24	n-undecane	a
	<b>nC12h26</b>	<b>C12H26</b>	<b>n-dodecane</b>	<b>b</b>
iso-alkane	<b>iC8H18</b>	<b>C8H18</b>	<b>iso-octane</b>	<b>c</b>
	iC12h26	C12H26	iso-dodecane	d
	<b>hmn</b>	<b>C16H34</b>	<b>iso-cetane</b>	<b>e</b>
cycloalkane	<b>C9h18-1</b>	<b>C9H18</b>	<b>propyl-cyclohexane</b>	<b>f</b>
	C10H20-1	C10H20	butyl-cyclohexane	g
	mC11h22	C11H22	pentyl-cyclohexane	h
aromatic	TMB124	C9H12	1,2,4-trimethylbenzene	i
	<b>t135mb</b>	<b>C9H12</b>	<b>1,3,5-trimethylbenzene</b>	<b>j</b>

Surrogate species chemical structure



Gen 2

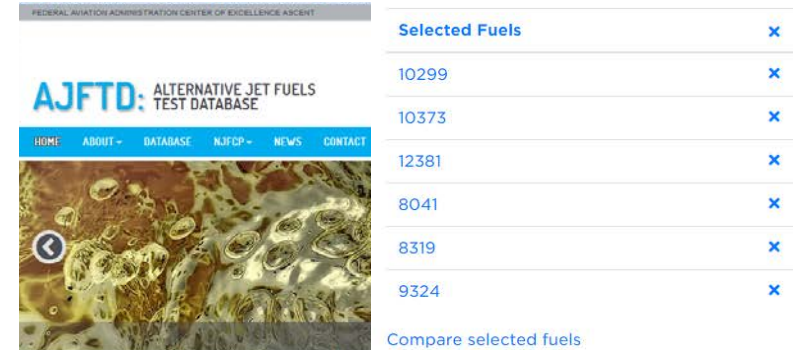


Results indicate F-24 fuel characteristics control LTC and improve AJF blend reactivity

# This work delivers the following key contributions

First dynamic jet  
fuel data resource

Disseminate  
critical fuel  
property data



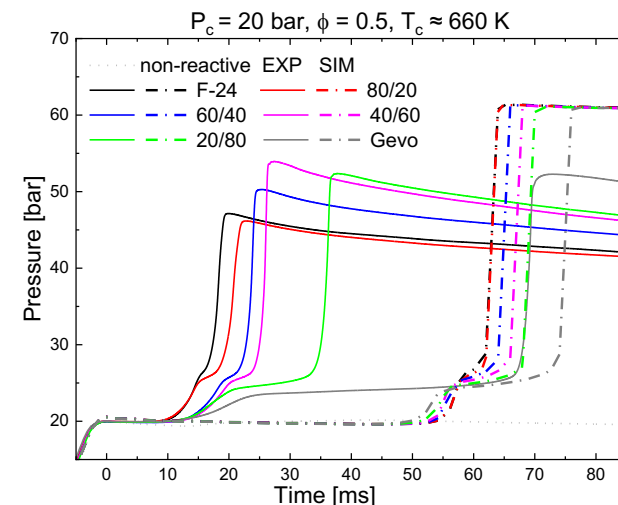
Novel AJF  
thermophysical &  
composition-  
property relations

Support fuel  
pre-screening  
& streamlining

Fuel Property	Significant Variance
Density	SKA
Isentropic Bulk Modulus	HEFA, FT
Specific Heat	FT, FSJF
Speed of Sound	HEFA
Viscosity	SKA, HEFA

Unique  
autoignition  
testing & kinetic  
modeling

Analyze fuel  
performance  
at low  $T$ , lean  
conditions





# AJFTD is first national platform to store and disseminate jet fuel research



***altjetfuels.illinois.edu***



Expanded Airport COA



Data Management



Upstream/Downstream Processes



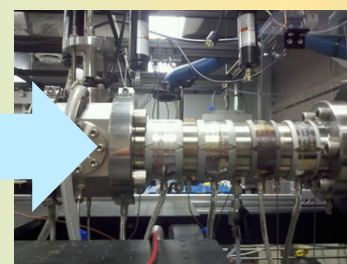
International Collaborations



Feedstock production & logistics



Conversion, scale-up & processing



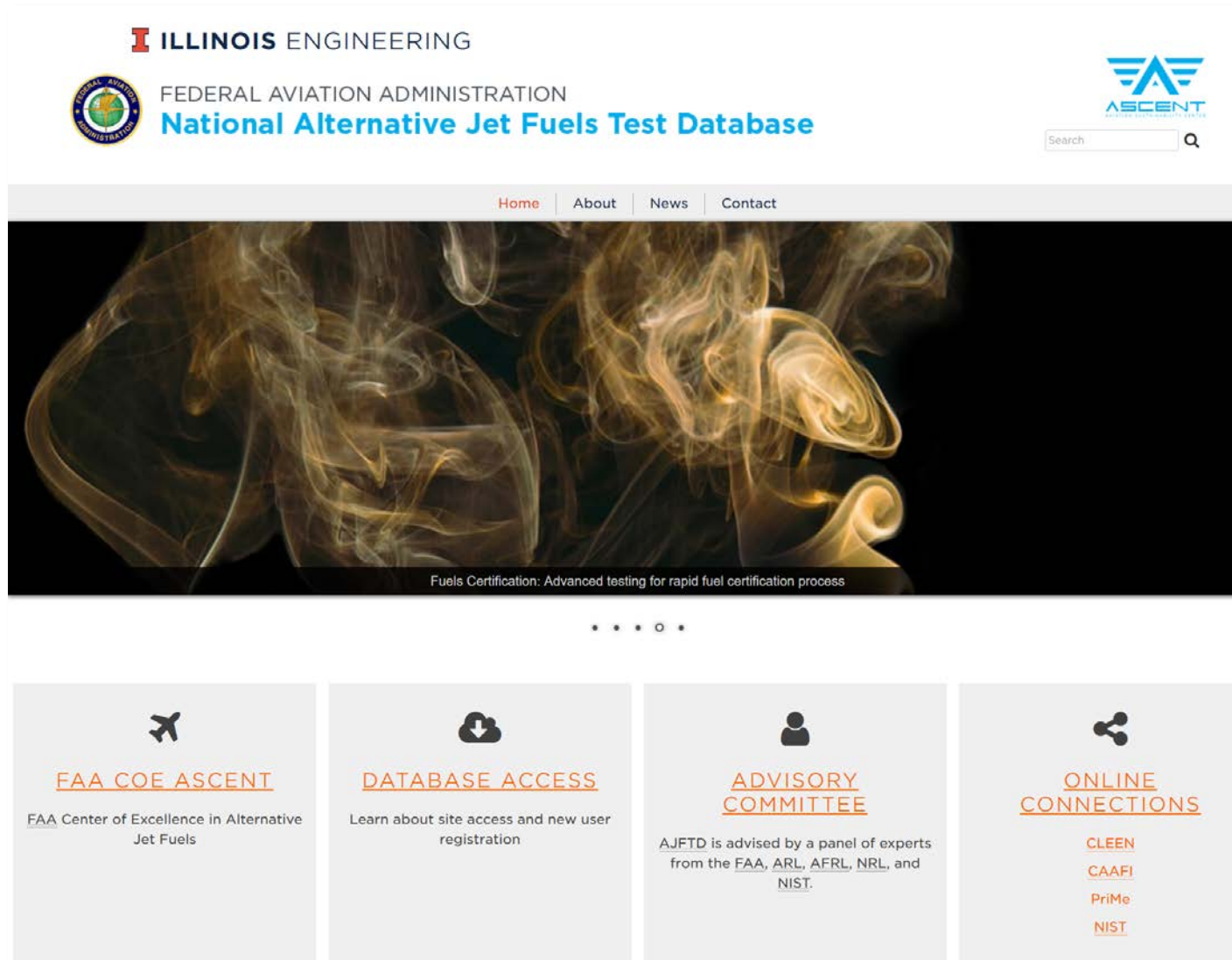
Fuel property testing & approval



End use production & emission testing

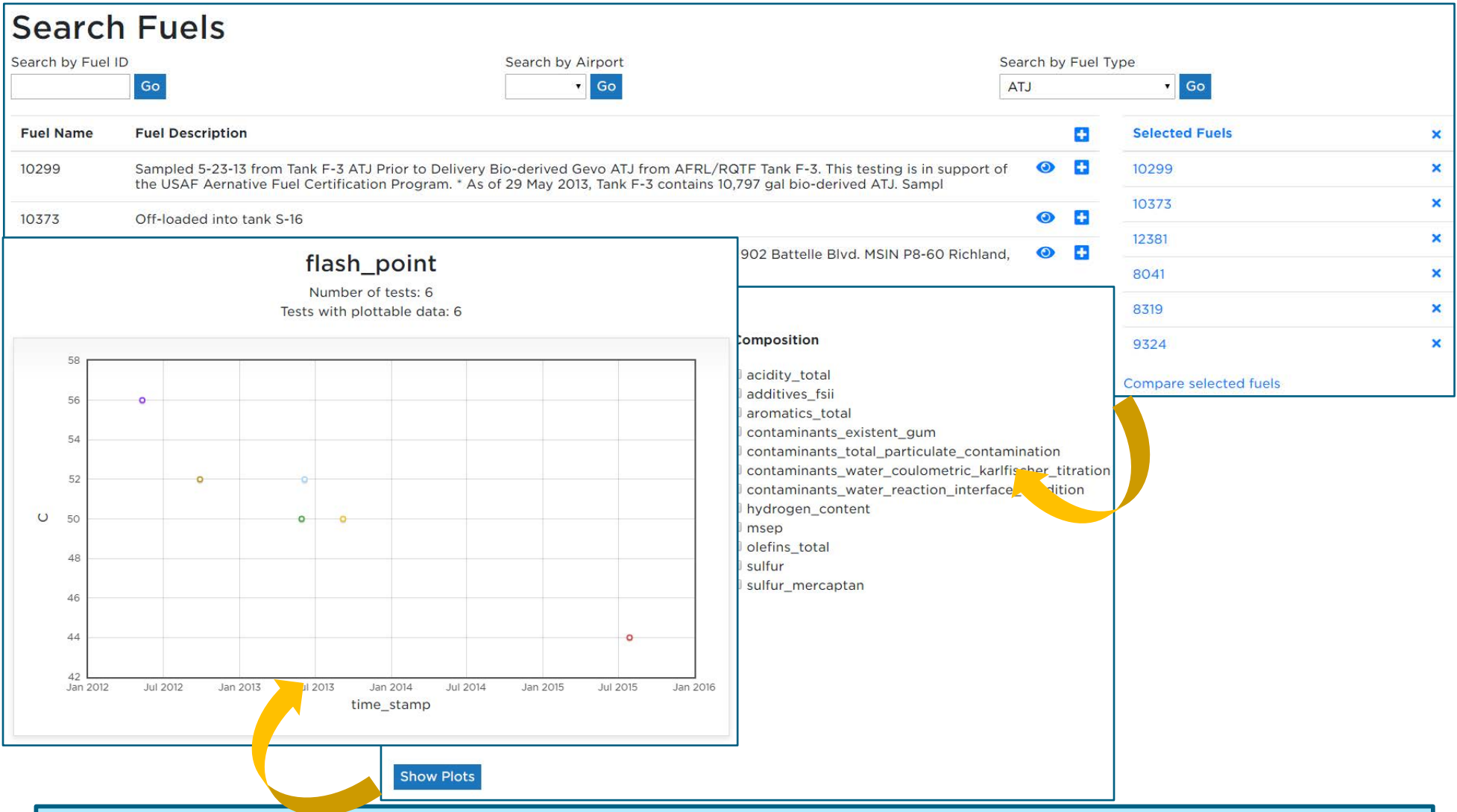
Critical for collaboration in fuel research community

# Gen II database – under development



- Same log-in authorization
- **Data submission** available for users
- Improved search result accessibility
- **Non Relational Data Analysis Interface**

# Gen II upgrades directly interface with database



AJFTD moved beyond file repository to interactive data tool



Coordinator:

**DLR**

Contact persons:

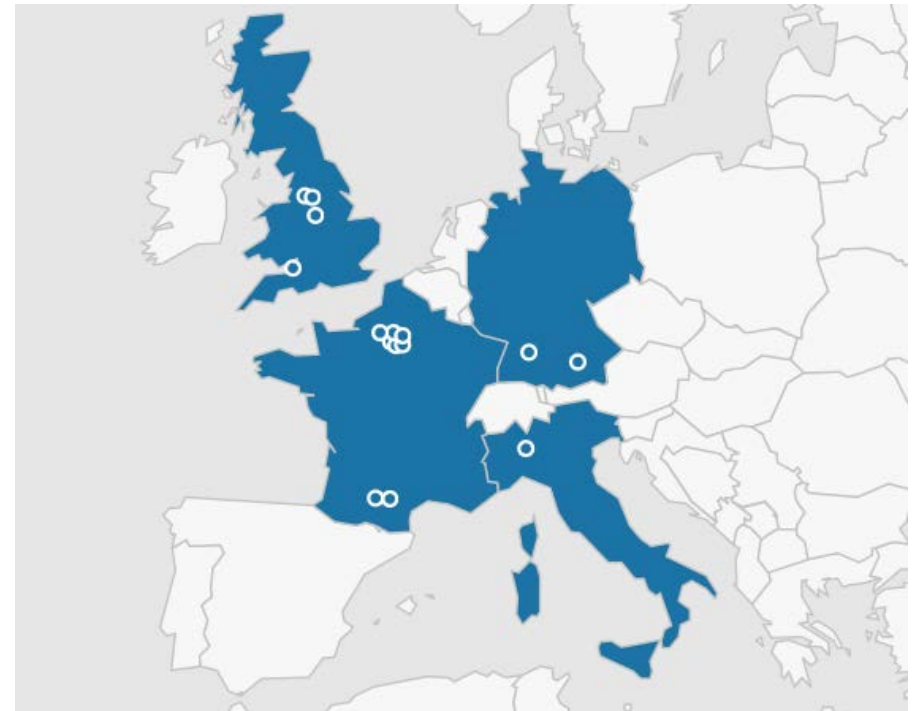
**Patrick Le Clercq and  
Bastian Rauch**

Address:

Pfaffenwaldring 38-40  
D-70569 Stuttgart  
GERMANY

Email:

**maroto@arttic.eu**



A project gathering **15 partners** from **4 European countries**:



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 723525

# Joint database vision - FAA & JETSCREEN



*One integrated database* with associated proprietary dataset (when necessary) containing:

- Detailed datasets from fuels world wide using common schema
  - Data range: conventional and alternative fuels, neat and blends
- **Task: Development of common database interface**
  - Different access levels depending on user group (Security)
  - Common interface to data but using different database backends (Mongo DB, DynamoDB) for the two databases
- **Task: Development & application of analysis tools with relevant stakeholders**
  - Different analysis tools based on programming platform and user needs
    - Employ specification property focused, performance centered, and/or end-use/ emissions targeted tools
  - Similar analysis strategy for both programs regarding key metrics



# Joint database provides access to expanded fuel dataset



Span **wide set of properties** (Tier 1 – Tier 4, fuel impact)

**Enable progress** in different areas:

## Safety & Reliability

**Coordinate fuel data** with

Global Aviation Data Management

- Track flight/ system issues with fuel information
- Investigate any fuel-related component failures

## Connect AJF & flight data

(maintenance records)

- Show safety & compatibility of AJFs with existing systems
- Increase market support for continued integration

## Expand fuel & flight records

- Increase safety for all participants

## Operations

**Track fuel properties in use:**

processing, supply chain, end use

- Improve quality control in fuel production & supply

Make **blend data accessible to airports & airlines**

- Demonstrate safe usage of AJFs with detailed supply info
- Build trust between producers, suppliers, & consumers

**Expand fuel operational data** compilation & dissemination

- Increase system optimization across industry

## Engineering/Science

**Statistical analysis** for aircraft-related properties

- Facilitate design of components impacted by fuel

**Model development & validation**

- Streamline approval, reduce early stage testing
- Enhance development & production of AJFs

# Acknowledgements



## *Support*

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